

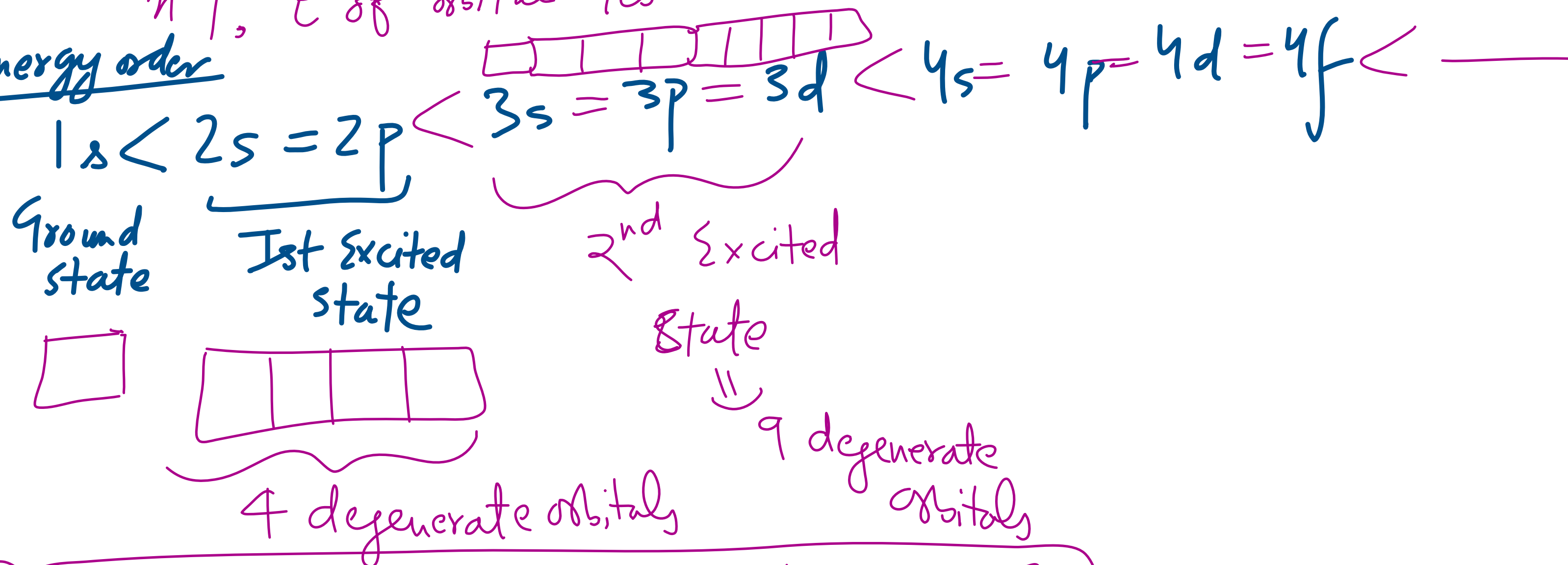
Energy order of orbitals

(i) Single electronic species ($\text{H}, \text{He}^+, \text{Li}^{2+}, \text{Be}^{3+}, \dots$)

E depends only on value of $n \Rightarrow$ shell No.

$n \uparrow, E \text{ of orbital } \uparrow$

Energy order



No. of degenerate orbitals in n^{th} shell $= n^2$

(2) for multielectron species (atom or ion)

Energy depends on both n & l value

Bohr-Bury Rule (n+l Rule)

$E \propto (n+l)$ value

If for any two orbitals, $(n+l)$ value is same, then

$E \propto n$

Energy order: $1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s$

(n+l) values:

1s	2s	2p	3s	3p	4s	3d	4p	5s
1+0	2+0	2+1	3+0	3+1	4+0	3+2	4+1	5+0
=1	=2	=3	=3	=4	=4	=5	=5	=5

eg: $\text{H}^{\oplus} \Rightarrow 2e$

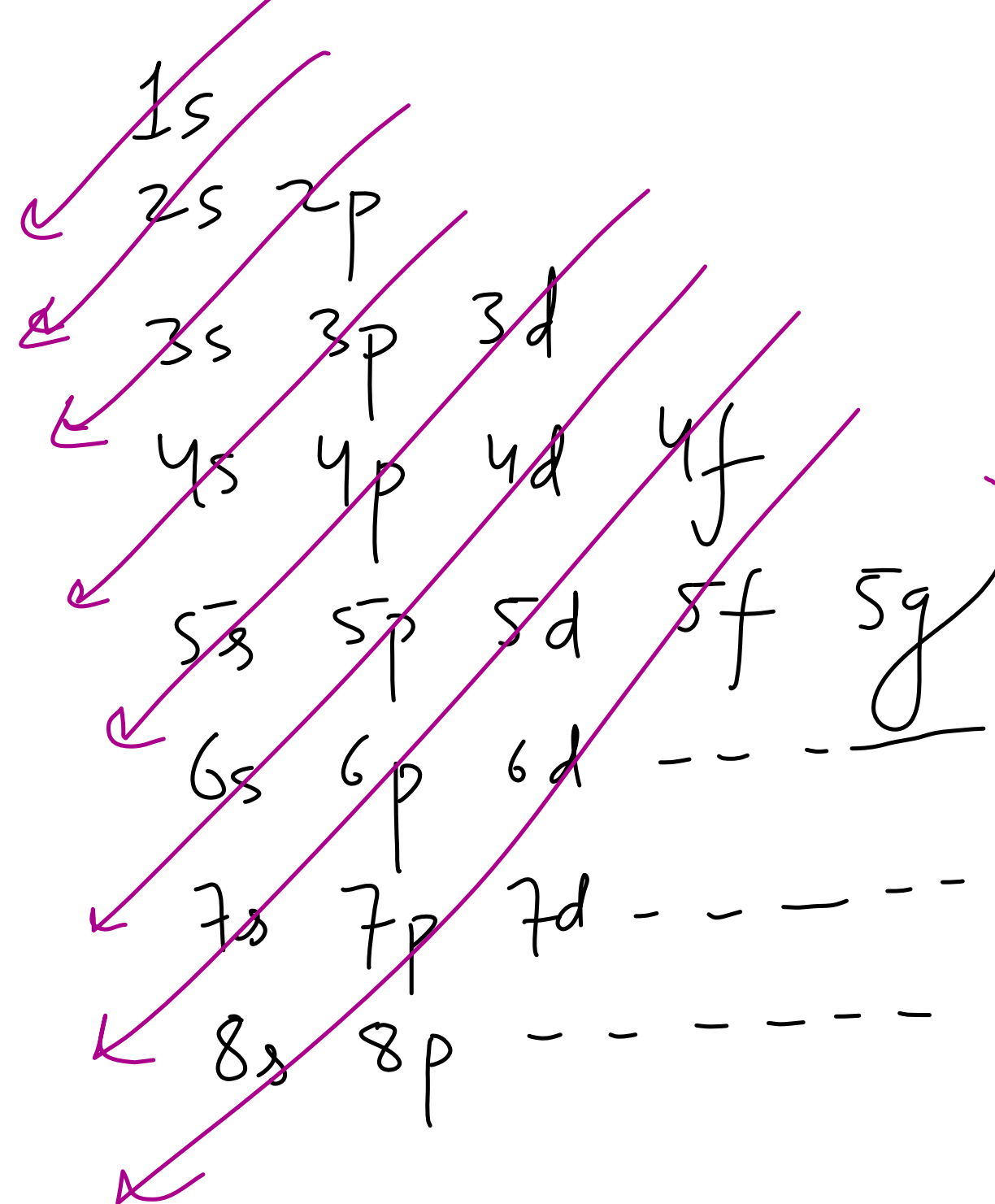
$\text{H}^{\oplus} = 1s^2$

Diagram showing orbitals and degeneracy:

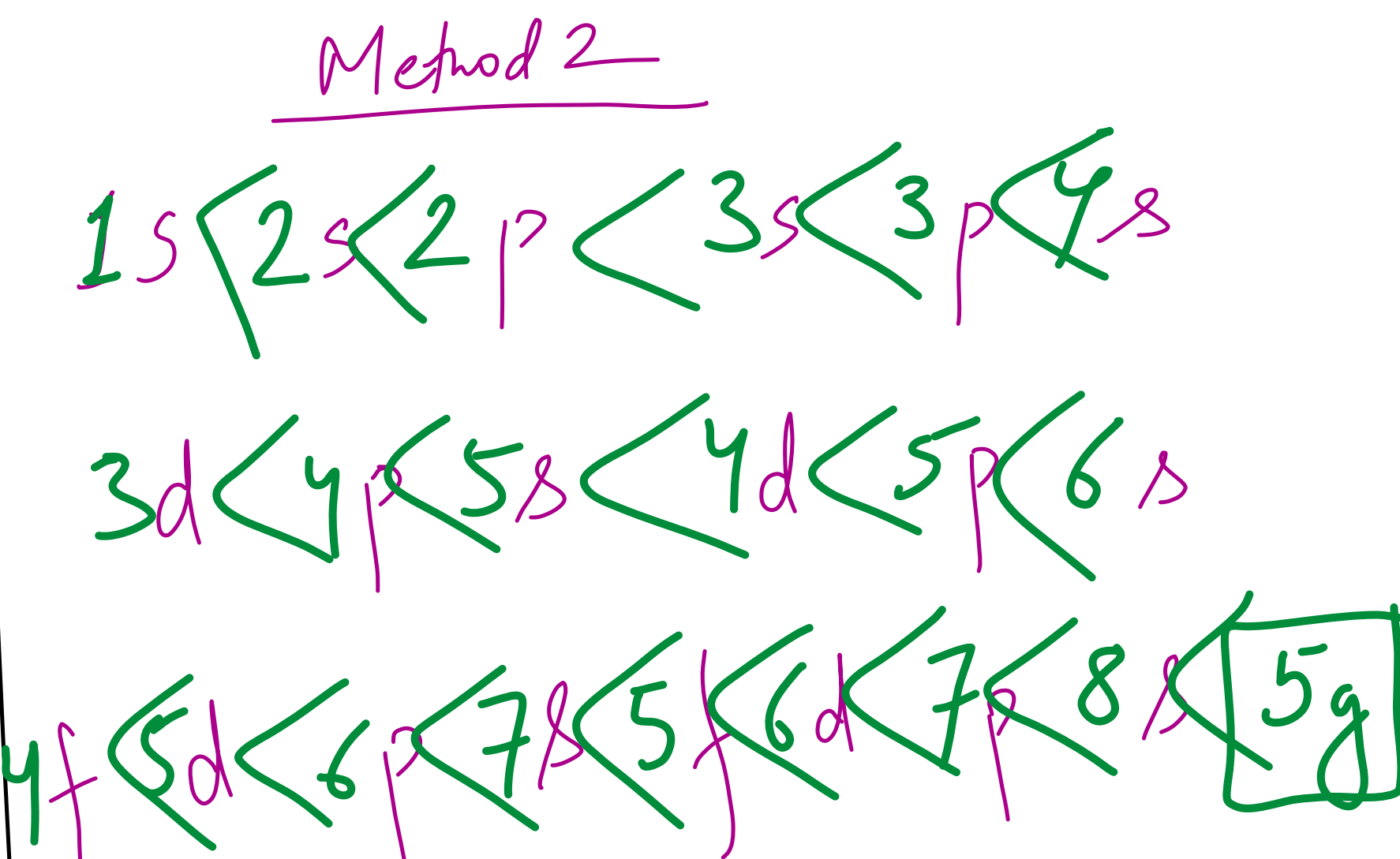
- 1s (1 orbital)
- 2s (1 orbital)
- 2p (3 degenerate orbitals)

#

Method 1



Method 2



Filling of e⁻s in orbitals

Rules

(I) Aufbau's Principle

"orbital having lower energy is filled before orbital having higher energy."

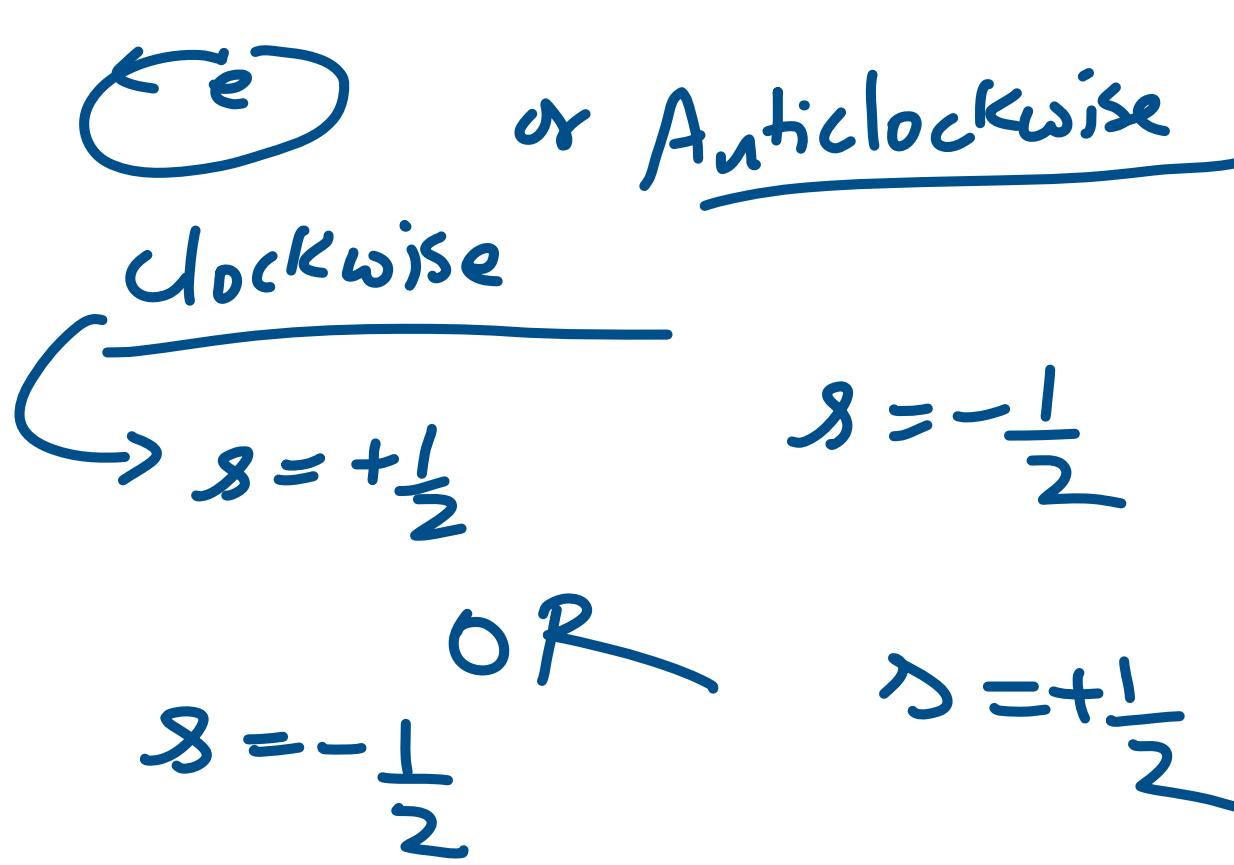
or
orbitals are filled in \uparrow ing order of their energy.

eg: 4th Quantum No. (Spin)

Not derived from Wavefunction

Spin Quantum No. (s) $\Rightarrow (\frac{1}{2})$

Each e^- revolves about its own axis



spin of e^- is represented as



(II) Hund's Rule of Maximum Multiplicity

Degenerate orbitals are first singly filled with same parallel spin (clockwise or anticlockwise) & then these e^- s are paired with opposite spin such that Maximum spin Multiplicity is achieved.

Spin Multiplicity (M_s)

$$M_s = 2|S| + 1$$

$$|S| = \text{Total Spin} = \sum s$$

eg: p^2

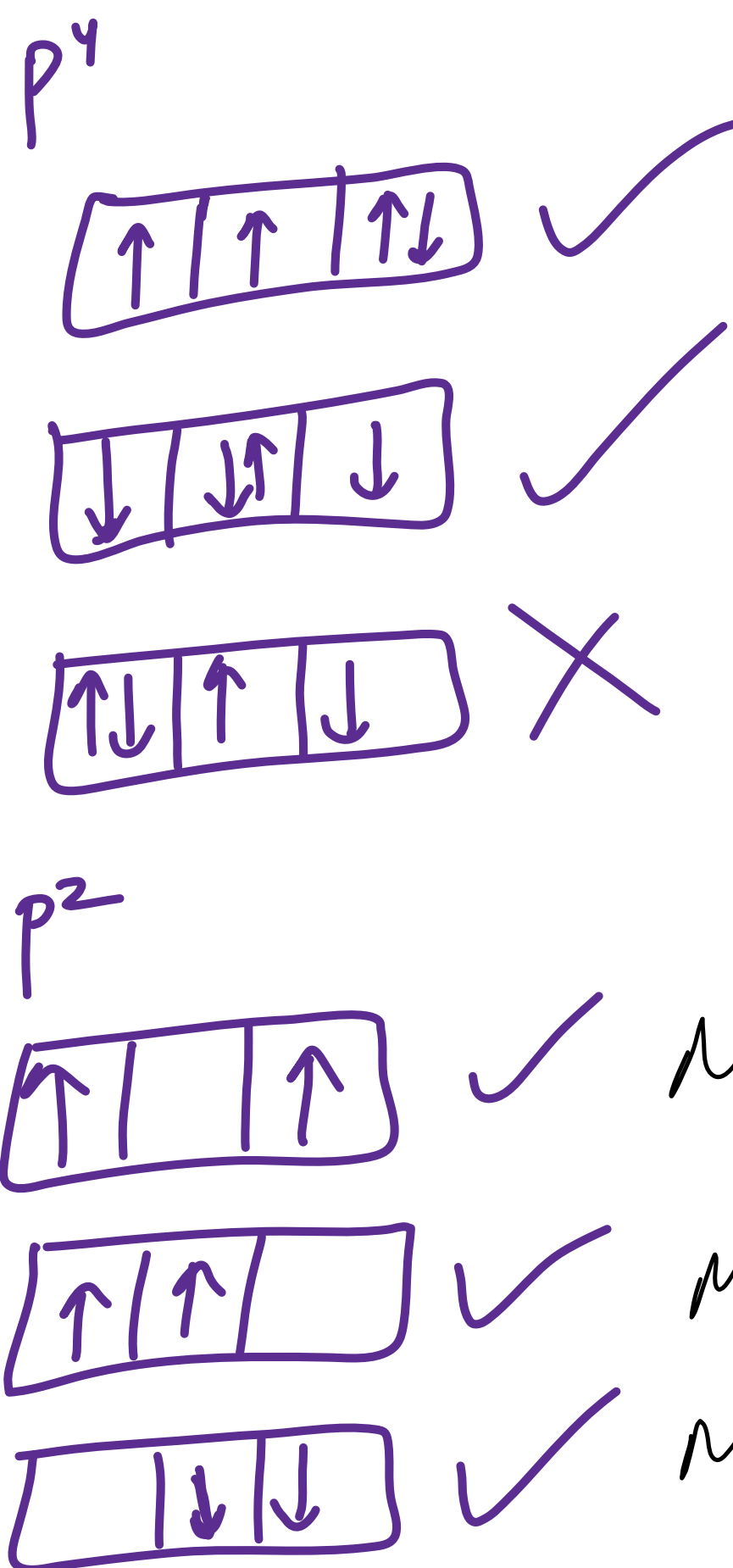
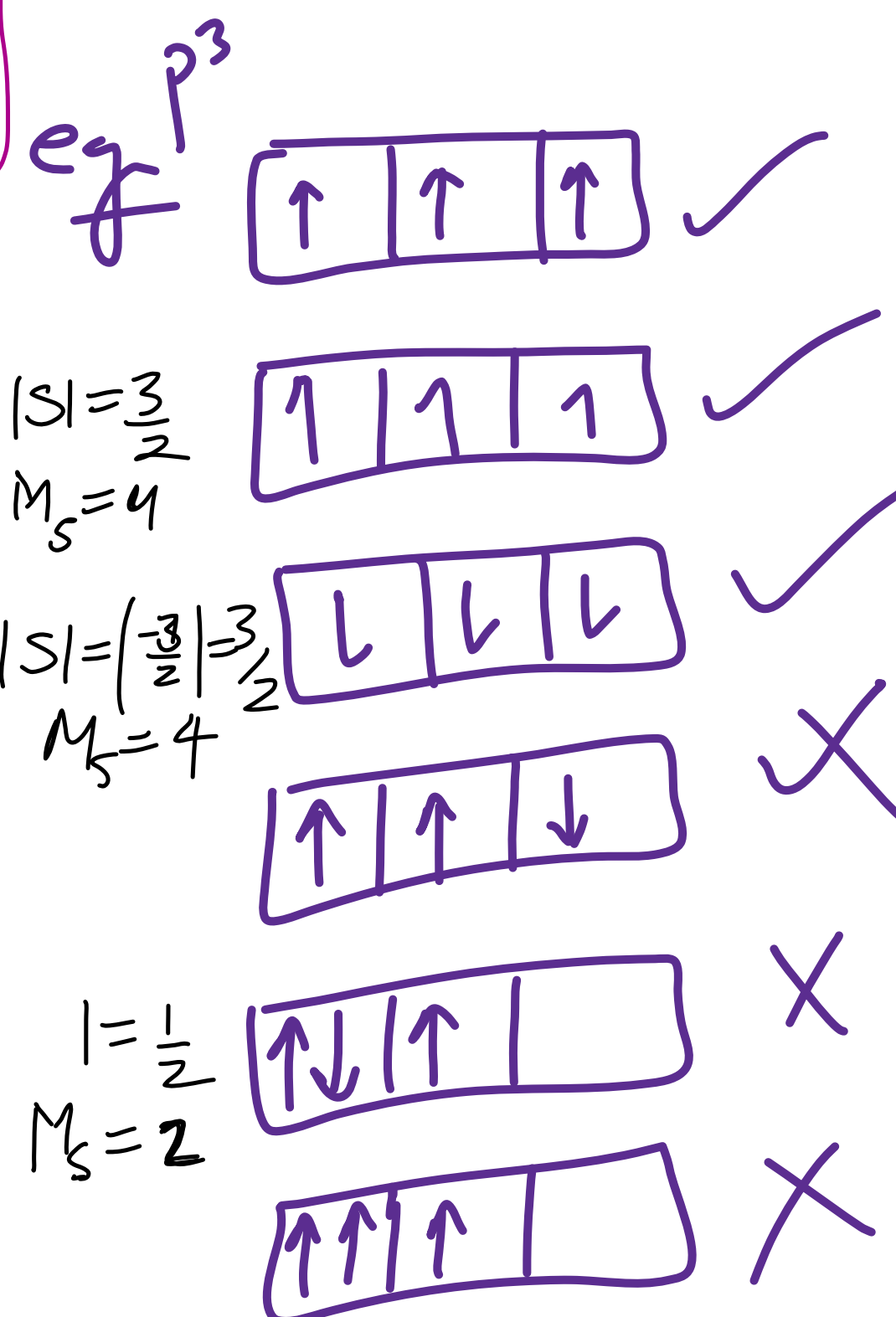
Diagram showing spin of p^2 :

- $\uparrow \uparrow$ (parallel spin)
- $|S| = |\frac{1}{2} + \frac{1}{2}| = 1$
- $M_s = 2 \times 1 + 1 = 3$

eg: p^2

Diagram showing spin of p^2 :

- $\uparrow \downarrow$ (paired spin)
- $|S| = 0$
- $M_s = (2 \times 0) + 1 = 1$



spin Angular Momentum of one e^-

$$= \sqrt{s(s+1)} \frac{h}{2\pi}$$

$$= \sqrt{\frac{1}{2}(\frac{1}{2}+1)} \frac{h}{2\pi}$$

$$= \frac{\sqrt{3}}{2} h$$